Equilibrium shapes and high-spin properties of the neutron-rich $A{\approx}100$ nuclei

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Abstract

Shapes and high-spin properties of nuclei from the neutron-rich ($N{>}56$) zirconium region are calculated using the Nilsson-Strutinsky method with the cranked Woods-Saxon average potential and monopole pairing residual interaction. The shape coexistence effects and the competition between rotationally-aligned $1h_{11/2}$ neutron and $1g_{9/2}$ proton bands is discussed. Predictions are made for the low-lying superdeformed bands in this mass region, characterized by the intruder states originating from the $\mathcal{N}{=}5$ and 6 oscillator shells.

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I. INTRODUCTION

Nuclei from the heavy-Zr region ($Z\sim40$, $N>56$) exhibit a wealth of structure phenomena such as, shape coexistence effects, dramatic variations in quadrupole collectivity, strong octupole correlations, and the existence of low-lying intruder states [1–3]. Most nuclei from this region are on the neutron-rich side and, therefore, they are not accessible using the standard in-beam techniques. The heaviest known isotopes in the A$\sim$100 mass region, namely ^{105}Y, ^{107}Zr, ^{110}Nb, ^{112}Mo, ^{115}Tc, and ^{117}Ru, have recently been observed [4] using the technique of in-flight isotopic separation of projectile fission fragments at relativistic velocities. Properties of β-decay of ^{103}Y, ^{105}Zr, ^{110}Nb, ^{110}Mo, ^{113}Tc, and ^{115}Ru, have been studied [5,6] at the IGISOL facility. These nuclei determine the present experimental spectroscopic boundary of this region.

A powerful tool to carry out spectroscopic studies in the neutron-rich systems is to analyze the prompt gamma rays from nascent fission fragments. In such measurements it is possible to approach *spectroscopically* very neutron-rich nuclei such as ^{102}Sr, ^{104}Zr, ^{108}Mo [7,8], and ^{112}Ru [9]. Rotational structures in this region have also been studied using breakup fusion reactions [10], (t,p) reactions [11], heavy-ion-induced fusion [12], incomplete fusion [13], neutron-induced fission [14,15], and deep inelastic reactions [16,17].

In spite of many experimental efforts, detailed information on high-spin properties of $A\sim100$ nuclei is still scarce. The first systematic study of high-spin states in even-even nuclei, as well as odd-A nuclei in this region, was reported in Ref. [8]. In the even-even Zr and Mo isotopes, the yrast lines are known up to I^π=12$^+$ [18–20]. In several nuclei such as ^{102}Ru [10], ^{104}Ru [16], $^{108-112}$Ru [9], and ^{104}Mo [16], a crossing between the ground band (g-band) and the aligned band (s-band) has been observed. Also, in a number of Ru and Mo isotopes, side-bands have been studied [9,14,21–23]. High-spin states in odd-A nuclei have been found in ^{101}Sr [24], ^{101}Zr [25], ^{103}Zr [26], ^{101}Nb [27], ^{103}Nb [28], ^{103}Mo [29], ^{105}Mo [30], ^{103}Rh [31], and ^{109,111}Ru [32]. For the heavy Sr isotopes, spectroscopic studies [33,34] are still in a preliminary stage, and practically nothing is known on the neighboring Kr and Se nuclei. It is conceivable that with the help of the new generation gamma-ray arrays such as GammaSphere and EuroBall, and with the help of radioactive beam facilities, the borders of the heavy-Zr regions will soon be expanded towards even heavier systems.

The strong dependence of observed spectroscopic properties on the number of protons and neutrons, makes the neutron-rich $A\approx100$ nuclei a very good region for testing various theoretical models. According to the mean-field-based calculations, strong shape variations in this region may be attributed to shell effects associated with large spherical and deformed subshell closures in the single-particle spectrum. The single-particle diagram, representative of the nuclei from the heavy-Zr region, is shown in Fig. 1. The strongest shell effects are expected for a spherical shape with the magic numbers 28, 50, and 82, and also for the subshell closures at Z=40 and N=56. The transition to a deformed region occurs near N=58 and 76; the strongest shell polarization towards deformed shapes is predicted for N=60-72. Finally, the best candidates for superdeformed shapes are nuclei with particle numbers near 42 and 64. [Shell-correction landscapes for the Zr-region are shown, e.g., in Ref. [35] (folded-Yukawa model), Ref. [36] (Woods-Saxon model), and Refs. [37,38] (Nilsson model).]

According to calculations based on the mean-field approach, the occupation of $1h_{11/2}$

neutron and $1g_{9/2}$ proton orbitals is essential for understanding the deformed configurations around ^{100}Zr [39]. The best examples of shape coexistence in this region are Sr, Zr, and Mo isotopes with $N{\sim}58$. In the language of the deformed shell model, the onset of deformation around N=58 can be associated with the competition between the spherical gaps at Z=38, 40, and N=56, and the deformed subshell closures at $\beta_2{\approx}0.35$ at particle numbers Z=38, 40, and N=60, 62, and 64. Theoretically, the delicate energy balance between spherical and deformed configurations depends crucially on the size of these gaps in the single-particle energies. As discussed in Refs. [40–42] the deformation onset at $N{\approx}58$ results from the subtle interplay between the deformation-driving neutron-proton energy (varying smoothly with the shell filling) and the symmetry-restoring monopole energy responsible for the shell effects.

Equilibrium deformations and moments, potential energy surfaces, microscopic structure of coexisting configurations, and shape transitions in the heavy-Zr region have been calculated by many authors [35–85]. In most cases, calculations show large deformations in Sr, Zr, and Mo isotopes with $N{\geq}60$. However, the details of the shape transition near N=58 is predicted differently by various models, the onset and rapidity of this transition being very sensitive to the model [2].

One of the most interesting features of nuclei from the $A{\sim}100$ region is the richness of various structural effects that occur at high angular momenta. Many of these effects have a straightforward interpretation in terms of the interplay between deformation, pairing, and the Coriolis force. In the deformed nuclei near ^{102}Zr, the alignment pattern is expected to be rather simple. While the first proton crossing can be associated with the breaking of the $1g_{9/2}$ pair, the lowest neutron crossing is due to the $1h_{11/2}$ alignment.

For even-even systems, band crossings have been seen in the g-bands of $^{108-112}$Ru [9], the N=60 isotones ^{104}Ru [8,10,16,17] and ^{106}Pd [86], the N=58 isotones ^{100}Mo [8,16], ^{102}Ru [10], and ^{104}Pd [86], and the N=56 isotone ^{100}Ru [87]. For proton numbers $Z{\geq}46$ the interplay between $1g_{9/2}$ protons and $1h_{11/2}$ neutrons is well established [88,89]. In the case of ^{102}Ru, the $1h_{11/2}$ neutron crossing is supported by blocking arguments in neighboring odd-N and odd-Z nuclei [10,31]. Namely, in the N=58 nucleus ^{103}Rh there is a clear crossing in both π=− and π=+ 1-q.p. proton bands, as well as in the 1-q.p. π=+ bands in ^{101,103}Ru. However, no crossing has been observed in the π=−, $1h_{11/2}$ bands in ^{101,103}Ru. Similarly, the presence of a band crossing in the yrast line of even-even nuclei ^{104}Ru and ^{104}Mo [16], and its absence in the π=− 1-q.p. bands in the neighboring odd-N systems, suggest that $1h_{11/2}$ neutrons are involved.

In addition to blocking arguments, there exists other experimental evidence for the presence of the $1h_{11/2}$ neutron unique-parity states in this mass region, notably the *direct* observation of negative-parity, very collective bands in ^{101,103}Zr, assigned to the [532 5/2] ($1h_{11/2}$) Nilsson orbital [7,18,25].

In the Ru and Mo isotopes with $N{\geq}60$, the role of (static or dynamic) triaxial shape degrees of freedom has been discussed. In $^{104-108}$Mo and $^{108-112}$Ru, the excitation energies of the 2^+_γ bandheads are low. Furthermore, in the ^{104,106}Mo isotopes, the band built upon the excited I^π=4$^+$ state, a candidate for the double-γ vibrational excitation, has been observed [22,23]. On the other hand, based on the energy differences and the $E2$ branching ratios analysis, triaxial deformations have been suggested for $^{108-112}$Ru [14]. The development of triaxiality at high spins has been addressed by measurements of γ-band→g-band branching

ratios [9] and by lifetime measurements [19,20].

Little is known about shapes of lighter elements in this region. Recent laser measurements of isotope shifts in the heavy Kr isotopes [90,91] indicate the absence of a sudden shape transition around N=60.

The main objective of this study is to investigate the importance of shape changes and pairing correlations in the description of high-spin bands in nuclei near ^{102}Zr. Predictions have been made for those nuclei which show the best prospects for triaxial shapes and for superdeformed bands at relatively low excitation energies.

The paper is organized as follows. The Woods-Saxon model and the total routhian surface technique are described in Sec. II. The results of ground-state calculations in the $A\sim100$ region are given in Sec. III. In particular, ground-state equilibrium deformations and their dependence on the treatment of pairing correlations and macroscopic energy are discussed. Cranking calculations are presented in Sec. IV, together with the analysis of typical alignment patterns, band structures, and shape changes. The summary and conclusions are contained in Sec. V.

II. THE MODEL

The macroscopic-microscopic method employed in this work is an approximation to the HF approach [92,93]. Its main assumption is that the total energy of a nucleus can be decomposed into two parts,

$$E = E_{\rm macro} + E_{\rm micro}, \tag{1}$$

where $E_{\rm macro}$ is the macroscopic energy and $E_{\rm micro}$ is the microscopic energy (shell correction) calculated from a non-self-consistent average deformed potential.

The shell corrections were obtained using the deformed Woods-Saxon (WS) potential of Ref. [94]. For the macroscopic energy, two energy formulas were employed: the liquid-drop (LD) model of Ref. [95] and the Yukawa-plus-exponential model (finite-range liquid-drop (FRLD) model) of Refs. [96,97]. The latter model is softer to shape distortions and, consequently, is expected to favor more deformed nuclear shapes [98–100].

The nuclear surface was defined by means of the standard multipole expansion,

$$R(\Omega) = c(\alpha)R_0\left[1 + \sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\Omega)\right], \tag{2}$$

with $c(\alpha)$ being determined from the volume-conservation condition and $R_0 = r_0A^{1/3}$. [Axial deformations β_λ are defined as $\beta_\lambda \equiv \alpha_{\lambda 0}$.]

In our analysis of equilibrium shapes we did not consider the odd multipolarity deformations. We are mainly interested in the dominant features related to the leading quadrupole effects. Secondly, as discussed previously [98,101], the static octupole deformations are not expected to be present in well-deformed neutron-rich $A\sim100$ nuclei.

The shell correction was calculated according to the prescription given in Ref. [93]. The results of the calculations presented in this paper were obtained with a smoothing width of $49.2/A^{1/3}$ MeV and a sixth-order curvature correction. All single-particle states lying below

a cut-off energy of $131.2/A^{1/3}$ MeV above the Fermi level were included. Our calculations are based on a three-dimensional minimization on the mesh, and the variation of the average potential with Z and N has been suppressed (i.e., the calculations were performed using single-particle energies of a representative central nucleus). The related errors in energy surfaces introduced by this procedure are known to be small [102].

In the I=0 calculations, pairing energies were computed using either the standard BCS treatment or the particle number projection method before variation (PNP). The latter method is expected to be more precise and reliable in the regions of low single-particle level densities where the BCS treatment breaks down. For the pairing calculations we took the lowest Z or N single-particle orbitals for protons or neutrons, respectively, counting from the bottom of the potential well. The pairing strengths were determined using the average gap method. The optimal choices for the average gap parameterization, discussed in Ref. [103], are adopted for this study. Namely, in the PNP variant we used average gaps of $\tilde{\Delta}_n = 8.6/\sqrt{A}\,\text{MeV}$ and $\tilde{\Delta}_p = 9.9/\sqrt{A}\,\text{MeV}$, and in the BCS variant we used $\tilde{\Delta}_n = 13.3/\sqrt{A}\,\text{MeV}$ and $\tilde{\Delta}_p = 13.9/\sqrt{A}\,\text{MeV}$.

The parameters of the WS potential were taken from Ref. [36]; however, they were adjusted to describe the rapid shape transition between ^{96}Zr and ^{100}Zr. These parameters differ from the standard set [104] only in the values of the spin-orbit potential strength. Namely, we adopted the values $\lambda_{\rm so,n}$=39 and $\lambda_{\rm so,p}$=32 instead of the standard values $\lambda_{\rm so,n}$=35 and $\lambda_{\rm so,p}$=36, respectively.

In order to study the variations of potential energy surfaces at I=0 (Sec. III), three sets of calculations were performed:

V1 Axial calculations in a three-dimensional deformation space (β_2, β_4, β_6). They were carried out by setting up a three-dimensional mesh with the mesh steps equal to 0.05 0.04, and 0.04 for β_2, β_4, and β_6, respectively. In these calculations we employed both LD and FRLD models for the macroscopic energy and both pairing models, i.e., BCS and PNP.

V2 The explicit energy minimization in a three-dimensional deformation space (β_2, β_4, β_6) performed for each isotope separately (here no assumption about a "central nucleus" has been made). In these calculations, we used the set of WS parameters of Ref. [36], the FRLD macroscopic energy, and the Lipkin-Nogami (LN) approximation to the PNP method (with the same pairing strengths as for the PNP mesh calculations). The details of the LN treatment are given in Ref. [102].

V3 Triaxial calculations in a three-dimensional deformation grid (β_2, γ, β_4). The mesh consisted of 10 points [0.05 (0.05) 0.50] in the $\beta_2\cos(\gamma+30^\circ)$ direction, 12 points [-0.20 (0.05) 0.35] in the $\beta_2\sin(\gamma+30^\circ)$ direction, and 4 points in the direction of β_4. To optimize the calculations, the β_4-grid was defined relative to the value of β_4 minimizing the LD energy at given β_2 and γ, $\beta_{4,\rm LD}(\beta_2,\gamma)$ [105]. Namely, the hexadecapole mesh was defined as $\beta_{4,\rm LD}(\beta,\gamma)+\Delta\beta_4$, $\Delta\beta_4$ being equal to –0.04 (0.04) 0.08. The hexadecapole deformation was included in a way which guarantees the modulo 60° invariance of the nuclear shape in the (β_2,γ) plane, i.e., the nonaxial hexadecapole deformations are present for γ not equal to multiples of 60° [98]. In this variant we employed the LD model for the macroscopic energy and both pairing models, i.e., BCS and PNP.

The high-spin behavior (I>0) of A∼100 nuclei was investigated using the total routhian surface (TRS) approach of Refs. [106,107]. The TRS cranking calculations were performed on a three-dimensional deformation mesh including β_2, γ, and β_4 deformations. The mesh was the same as that described in variant **V3**. The calculations were carried out for all nuclei with Z=38-44 and N=58-66, and for rotational frequencies $\hbar\omega$=0.075 (0.075) 1.50 MeV. The total routhians were defined as:

$$E^{\omega} = E^{\omega=0} + \langle \Psi^{\omega} \mid \hat{H}^{\omega} \mid \Psi^{\omega} \rangle - \langle \Psi^{\omega=0} \mid \hat{H}^{\omega=0} \mid \Psi^{\omega=0} \rangle, \tag{3}$$

where $E^{\omega=0}$ is the energy calculated at a given deformation according to the shell-correction method, $\hat{H}^{\omega}$=$\hat{H}$−$\omega\hat{j}_x$ is the total routhian including the pairing term, and $|\Psi^{\omega}\rangle$ is the independent quasi-particle vacuum at a given rotational frequency. Due to the size of this computation, the LD model was employed for the macroscopic energy. In our analysis of rotational bands, we limited ourselves to the vacuum configurations of even-even systems. That is, only the positive-parity, even-spin (signature r=1) bands were considered.

The average BCS pairing gap was parameterized in a way which facilitates separate calculation for neutrons and for protons: $\tilde{\Delta}_n = 4.93N^{-1/3}$ and $\tilde{\Delta}_p = 4.70Z^{-1/3}$ [103]. For nonzero spins the pairing gaps were parameterized as functions of rotational frequency:

$$\Delta(\omega) = \begin{cases} \Delta(0)\left[1 - \frac{1}{2}\left(\frac{\omega}{\omega_c}\right)^2\right], & \omega < \omega_c \\ \frac{1}{2}\Delta(0)\left(\frac{\omega_c}{\omega}\right)^2, & \omega > \omega_c \end{cases} \tag{4}$$

The parameter $\hbar\omega_c$ was fixed at 0.75 MeV for neutrons and 0.9 MeV for protons. The proton and neutron chemical potentials of the RBCS equations were adjusted at each deformation and rotational frequency separately so as to satisfy the particle number equation.

III. GROUND-STATE EQUILIBRIUM DEFORMATIONS

The potential energy surfaces (PES) for the neutron-rich even-even Kr-Pd isotopes obtained in the axial variant **V1** are shown in Figs. 2 and 3. The results of triaxial calculations (variant **V3**) are displayed for selected nuclei in Figs. 4 (^{100,102}Zr), 5 (^{104,106}Zr), 6 (^{100,102}Mo), 7 (^{104,106}Mo), 8 (^{104,106}Ru), and 9 (^{108,110}Ru).

The calculated equilibrium deformations obtained by means of the explicit minimization at axial shape (variant **V2**) are shown in Table I, and Table II displays the calculated equilibrium deformation obtained by a minimization in the (β_2, γ)-plane (variant **V3**).

A. General properties of potential energy surfaces

The modification of the WS parameters according to Ref. [36] has some impact only on the isotopes with N=56 and N=58; the optimized parameters tend to lower the PES around the spherical point. The most pronounced differences are obtained for the Sr and Zr isotopes where the equilibrium deformations are drastically changed. For other N=56, 58 isotones the equilibrium deformations are only slightly modified. More pronounced is the dependence on the choice of the macroscopic energy and on the pairing treatment. Namely,

the most pronounced minima and the largest equilibrium deformations were obtained in the FRLD/PNP model (Figs. 2 and 3). The LD/BCS variant yields rather shallow minima, especially for the Mo and Ru isotopes, and the smallest equilibrium deformations.

For most nuclei considered, the calculations predict two minima corresponding to prolate and oblate shapes. In the Kr, Sr, and Zr isotopes, these minima are separated by a relatively high spherical barrier. The largest prolate deformations cluster at the middle of the shell, i.e., around Z=38, 40, and N=60, 62, and 64. As discussed above, these particle numbers can be associated with large prolate gaps in the single-particle spectrum (see Fig. 1).

The barrier height (and the oblate-prolate) energy difference decreases with Z. As will be discussed below, in many cases the secondary minima are unstable to triaxial deformation. In the PNP calculations, there appear local substructures in the potential energy curves; the PES's calculated in the BCS variant are smoothed. The largest effects occur in the Mo isotopes where the prolate minimum splits into two components, and in the Ru isotopes with N=72-76, where secondary minima with large deformation $\beta_2 \approx$0.45-0.50 appear.

In triaxial calculations (**V3**), the Sr and Zr isotopes are predicted to be axial, while the Mo-Pd isotopes are calculated to be γ-soft. This is illustrated in the potential energy surface (PES) described in Figs 4, 5(Zr), 6, 7 (Mo), 8 and 9 (Ru). In the PNP variant, the PES's of the Mo isotopes with N=58, 60 show very shallow, γ-unstable valleys corresponding to β_2 ranging from 0.22 to 0.30. The heavier Mo isotopes with N=62-66 have shallow triaxial minima at $\gamma\approx 20^\circ$ and $\beta_2 \approx$0.32. All Ru isotopes have been found to be triaxial in their ground states, with shallow minima at $\gamma\approx 20^\circ$. Again, the minima calculated in the PNP variant are more pronounced than those in the BCS variant. (For more discussion on the influence of the PNP on the rigidity of the PES minima, see Refs. [61,108].)

B. Equilibrium deformations and quadrupole moments

The calculated equilibrium deformations obtained by means of the explicit minimization at axial shape (variant **V2**) are displayed in Table I, together with the predicted oblate-prolate energy differences, and calculated and experimental [109] intrinsic quadrupole moments. The oblate-prolate energy difference is defined as $\Delta E_{\rm op}$=$E_{\rm o}$–$E_{\rm p}$, where $E_{\rm o}$ corresponds to the minimum with negative β_2 while $E_{\rm p}$ corresponds to the minimum with zero or positive β_2. The quadrupole moments were extracted from the calculated equilibrium deformations using the procedure outlined in Ref. [102]. In Table II, the calculated equilibrium deformations obtained by means of the minimization in the (β_2, γ) plane are displayed, together with the calculated transition quadrupole moments, defined as [110]

$$Q(\gamma) = \frac{2}{\sqrt{3}} Q_0 \cos(\gamma + 30^\circ), \tag{5}$$

where Q_0=$Q(\gamma = 0^\circ)$.

It is instructive to compare the equilibrium deformations obtained in our work with those of Chasman calculated using the LD model and the shell correction approach with WS potential [64], those obtained by Möller *et al.* in the shell correction approach with the folded-Yukawa single-particle potential and the finite-range droplet-model (FRDM) [74], and with the results of the extended-Thomas-Fermi model (ETFSI) of Ref. [65].

The heavy Se isotopes are predicted to be oblate-deformed with $\beta_2 \approx -0.28$ and very large values of $\beta_6 \approx 0.10$. The prolate-deformed minima appear 0.4–1.4 MeV higher in energy. This result is consistent with the ETFSI calculations which yield oblate shapes with $\beta_2 = -0.31$ for all Se isotopes with $N>58$. On the other hand, FRDM favors prolate shapes with $0.29<\beta_2<0.33$.

The heavy Kr isotopes are predicted to be oblate-deformed ($\beta_2 \approx -0.31$, $\beta_6 \approx 0.10$) up to $N \sim 66$. For the Kr isotopes with $N>64$, $\Delta E_{\rm op}$ is rather small. This is due to the large oblate gap with $Z=36$. This result is consistent with the ETFSI calculations which yield an oblate-prolate shape transition at $N \approx 68$. The FRDM favors well-deformed prolate ground states with $\beta_2 \approx 0.33$. The recent laser-spectroscopy measurements [90,91] show that the observed $\langle r^2 \rangle$ does not drastically change at $N=60$, indicating that there is no sudden increase of $|\beta_2|$ for $N \leq 60$ nuclei. Since the deduced β_2 is ≈ 0.3 for $N=60$, all these calculations are consistent with this experiment.

The heavy Sr isotopes with $60 \leq N \leq 72$ are predicted to have well-deformed prolate ground states in all the models discussed. The calculated quadrupole deformations β_2 range from 0.30 to 0.40. Contrary to the FRDM results, both our calculations and those of the ETFSI model yield a rapid shape transition at $N \approx 56$.

The heavy Zr isotopes with $60 \leq N \leq 72$ are predicted to have well-deformed prolate ground states ($0.33 \leq \beta_2 \leq 40$) in all the models discussed. At $N \approx 74$, the transition to oblate shapes is predicted. This transition appears much earlier, at $N=66$, in the calculations by Chasman. The rapid shape change between $N=56$ and $N=60$ is reproduced by our model, by Chasman, and by the ETFSI model. In the FRDM, the shape change is calculated to be more gradual; the nucleus ^{96}Zr is predicted to be prolate-deformed with $\beta_2=0.2$ (see the discussion in Ref. [35] regarding the single-particle structure of the folded-Yukawa potential near ^{96}Zr). As seen in Figs. 5, the heavy-Zr isotopes with $N \geq 66$ become γ-soft.

In *the heavy Mo isotopes*, the calculated oblate-prolate energy difference decreases, hence the competition between low-lying coexisting minima is more pronounced. In contrast to the Sr and Zr isotopes, the transition from spherical to deformed shapes in the Mo isotopes at $N \approx 58$ is predicted to be gradual, in agreement with experimental findings. The transitional nucleus ^{102}Mo is very soft and the isotopes ^{104,106,108}Mo are calculated to have triaxial ground-state minima. Similar results were predicted by Chasman, in the Nilsson-Strutinsky calculations of Ref. [57], and in the Skyrme-Hartree-Fock study [55]. The prolate-to-oblate shape transition is expected at $N \approx$68-70 in all these models.

In *the heavy Ru isotopes*, the prolate-to-oblate shape transition is predicted at $N \approx 66$ in our axial calculations and in the FRDM, but much earlier, at $N \approx 60$, in the ETFSI model. Again, as in the Mo case, our calculations for the Ru isotopes predict γ-softness or triaxiality. Similar results were obtained by Chasman, by the Nilsson-Strutinsky calculations of Ref. [52], and by the Skyrme-HF study [21].

Stable triaxial shapes in $^{108-110}$Ru have recently been reported in Ref. [14]. Our calculations are consistent with the experimentally deduced γ values, namely 23° for ^{108}Ru and 24° for ^{110}Ru, but fail in reproducing the experimental quadrupole moments. That is, after correcting for the effect of triaxiality using Eq. (5), theoretical quadrupole moments for Mo and Ru isotopes are predicted to be too large. Interestingly, axial calculations reproduce measured values rather well (cf. Tables I and II), but they overestimate the experimental quadrupole moments for other systems predicted to have near-axial shapes. A possible source

of this discrepancy is the shape mixing phenomenon which gives rise to the fragmentation of the experimental low-lying $B(E2)$ strength.

IV. HIGH-SPIN CALCULATIONS

A. Total Routhian Surfaces: Examples

Figures 10, 11, and 12 show typical examples of total Routhian surfaces for nuclei from the heavy-Zr region. The nucleus ^{100}Sr, Fig. 10, represents a well-deformed collective rotor. The prolate minimum, β_2≈0.35, does not change significantly with angular momentum up to I≈36. Only at a very high rotational frequency does this minimum become triaxial (γ>0°) due to alignment of several high-j quasi-particles (see Sec. IV B). The coexisting oblate minimum (γ≈–60°) is also fairly stable with I.

In ^{102}Zr (Fig. 11) the situation is different. There is a shape change from the well-deformed prolate minimum to a triaxial minimum with γ<0° associated with the first band crossing. The local minimum at γ≈–60°, seen in the $\hbar\omega$=0.3 MeV surface, quickly becomes non-yrast with increasing ω. At very high rotational frequencies, the superdeformed (β_2≈0,4), slightly triaxial, minimum becomes yrast at I≈50.

The nucleus ^{108}Ru (Fig. 12) is representative of a γ-soft system. Here, the competition between several near-yrast triaxial minima produces dramatic shape changes. Although the triaxial minima are rather shallow at ω=0 (see Fig. 9), they become stabilized at high spins due to quasi-particle alignment. The superdeformed minimum with β_2≈0.5 appears at exceptionally low spins. At $\hbar\omega$=0.6 MeV, this minimum lies only ≈2 MeV above the triaxial yrast line.

B. Shape Changes at High Spin

The systematics of calculated equilibrium β_2 and γ deformations for even-even nuclei with N=58-66 are displayed in Figs. 13 (Sr), 14 (Zr), 15 (Mo), and 16 (Ru). All the local minima that appear in calculated TRS's are visualized as I-dependent trajectories in the (β_2, γ) space. In the following discussion, rotational bands and their underlying intrinsic configurations are grouped into several categories, according to their deformations and intruder content. In most cases, the dependence of equilibrium deformations on configuration and angular momentum can be simply explained in terms of two factors: (i) the deformation softness of the PES at I=0; and (ii) the position of the Fermi level, λ, relative to an intruder high-j shell. In this context, recall that the routhian of the strongest-aligned quasi-particle has a minimum as a function of γ that is strongly dependent on the position of λ within the shell. Namely, if the Fermi level lies at the bottom of the shell, positive values of γ are favored, for a half-filled shell γ≈–30° is preferred, and for λ in the upper half of the shell, the aligned high-j particle drives the core towards γ<–60° [111–114]. Of course, the total shape polarization exerted by aligned quasi-particles results from an interplay between the contributions of protons and neutrons.

1. Prolate shapes with $\beta_2 \approx$ 0.27-0.35.

The well-deformed prolate shapes are typical of ground-state rotational bands in Sr and Zr nuclei. As seen in Table I, ground-state deformations gradually increase from β_2≈0.28 in N=58 isotones to β_2≈ 0.33-35 in the heavier systems.

For all Sr isotopes except ^{104}Sr (N=66), the deformation of the aligned $(\nu h_{11/2})^2$ 2-q.p. configuration is nearly the same as that of the ground state band. Indeed, the calculated values of β_2 are only slightly reduced and the values of $|\gamma|$ are close to zero. For ^{104}Sr, the neutron Fermi level is higher in the $1h_{11/2}$ shell, i.e., between [532 5/2] and [523 7/2] orbitals (Fig. 1). Consequently the $(\nu h_{11/2})$ alignment is reduced and the $\nu h_{11/2}$ crossing is predicted at a rotational frequency close to that of the $(\pi g_{9/2})$ crossing.

The values of γ calculated for the $(\nu h_{11/2})^2(\pi g_{9/2})^2$ 4-q.p. configurations depend on N (see Fig. 13). This can be explained in terms of the polarizing effect of the aligned high-j particles. Indeed, for N=58 (bottom of the $\nu h_{11/2}$ shell), γ deformation of a 4-q.p. band is calculated to be positive, and with increasing N the system is driven to negative γ-values. Interestingly, this polarizing effect is not observed for the $(\nu h_{11/2})^2$ bands. This can be explained in terms of a rather γ-rigid potential of the vacuum configuration (g-band). The γ-driving force exerted by the aligned $(\nu h_{11/2})^2$ pair is not sufficient to polarize the system towards $\gamma\neq 0$. However, the additional deformation-driving effect of the aligned $1g_{9/2}$ protons is sufficient to make the system triaxial. As expected, the alignment of the second pair of $1h_{11/2}$ neutrons gives rise to a reduction of β_2 in the $(\nu h_{11/2})^4(\pi g_{9/2})^2$ 6-q.p. configuration. The exception to this pattern is ^{96}Sr where the *increase* in β_2 can be attributed to the $\nu g_{7/2}$ alignment.

The Zr isotopes are γ-softer than the Sr isotopes (cf. Figs. 10 and 11), and shape changes at high spins are more pronounced. The g-bands are predicted to be prolate. The deformation change is associated with the $1h_{11/2}$ neutron alignment. Indeed, as seen in Fig. 17, displaying the quasi-particle routhians characteristic of a well-deformed prolate g-band in ^{102}Zr, the proton $1g_{9/2}$ crossing frequency is higher than the neutron $1h_{11/2}$ crossing frequency. In most cases, the aligned $(\nu h_{11/2})^2$ bands are triaxial, with slightly negative γ values.

For some Sr and Zr isotopes, at large spins (I∼30–50) there appear prolate well-deformed minima with β_2∼0.32–0.38. The associated configurations are $(\nu h_{11/2})^4(\pi g_{9/2})^2$ and $(\nu h_{11/2})^4(\nu i_{13/2})^1(\pi g_{9/2})^2$ (see Fig. 17).

The experimental and calculated angular momentum alignment for the well-deformed near-prolate yrast bands of ^{100}Zr and ^{102}Zr are presented in Fig. 18. Although our calculations are adiabatic and hence unable to reproduce the alignment pattern in the band crossing region, it is clearly seen that the first band crossing is associated with the $\nu h_{11/2}$ alignment.

2. Triaxial or near-oblate collective minima with –75°$\lesssim\gamma\lesssim-$15°

In the heavy *Sr isotopes* there appear excited minima at oblate shapes which give rise to rotational bands (g′-bands) at γ=–60°. Except for the N=58 isotope (β_2=0.17), associated β_2 deformations are typically ≈0.25 and increase slightly with increasing I. The oblate bands are predicted to lie at $E^*\gtrsim$1 MeV above the yrast configuration. At higher spins, $I\gtrsim$20,

triaxial bands built upon several aligned quasi-particles $[(\nu h_{11/2})^2(\pi g_{9/2})^2$, $(\nu h_{11/2})^4(\pi g_{9/2})^2$, $(\nu h_{11/2})^4(\nu i_{13/2})^1(\pi g_{9/2})^2]$ emerge. Within these bands, β_2 values vary smoothly, from $\beta_2 \approx 0.3$ to ≈ 0.22. The triaxial many-quasi-particle bands extend over $I \approx 24$-46 for N=60 and 62, $I \approx 18$-52 for N=64, and $I \approx 30$-52 for N=66. They are highly excited ($E^* \gtrsim 2$ MeV above yrast).

The heavy *Zr isotopes* with N=58–62 are predicted to have oblate collective bands similar to those calculated for the Sr isotopes. For N=64 and 66, triaxial minima with negative γ deformations are predicted. The corresponding configurations are $(\nu h_{11/2})^2(\pi g_{9/2})^2$ and $(\nu h_{11/2})^4(\pi g_{9/2})^2$, extending from $I \approx 20$ to $I \approx 42$. In ^{106}Zr, a 8-q.p. $(\nu h_{11/2})^4(\nu i_{13/2})^1(\pi g_{9/2})^2$ band is predicted at high spins, $I \sim 50$. However, due to the large quasi-particle content, its collectivity is weak ($\beta_2 \approx 0.15$, $\gamma \approx -80^\circ$). The excitation energy of this band is 1-4 MeV above the superdeformed (SD) yrast band.

The heavy *Mo isotopes* are predicted to have triaxial g-bands with negative γ values. For N=58 and 60, the triaxial minima are very shallow. The large excursions in the γ direction shown in Fig. 15 are due to this softness (or γ-instability) and hence should not be taken literally. The heavier Mo isotopes have better localized triaxial minima ($\beta_2 \sim 0.3$, $\gamma \sim -20^\circ$). Consequently, the deformation changes in their g-bands are small. The quasi-particle routhian diagram, characteristic of triaxial configurations in Mo and Ru isotopes, is presented in Fig. 19. Figure 20 shows the experimental and calculated angular momentum alignment for the yrast band of ^{108}Ru. In contrast to the situation for prolate shape (Fig. 17), here the $\pi g_{9/2}$ alignment is expected to occur at a lower frequency. Because of the deformation softness, shape changes with quasi-particle alignment are more dramatic in the Mo isotopes than in their (more rigid) Sr and Zr isotones. In most cases, highly aligned bands have $\gamma \lesssim -30^\circ$, and their collectivity gradually decreases with I. For example, the $(\nu h_{11/2})^4(\nu i_{13/2})^1(\pi g_{9/2})^2$ and $(\nu h_{11/2})^4(\nu i_{13/2})^1(\pi g_{9/2})^4$ configurations calculated at $I \approx 40$-50, have weakly deformed shapes with $\beta_2 \approx 0.12$.

In recent experimental work [20], transition quadrupole moments of high-spin states in the neutron-rich Mo isotopes have been measured using the Doppler-profile method. The observed reduction of quadrupole moments at $I \approx 10$ has been interpreted in terms of a deformation change from axial shapes towards triaxial shapes with $\gamma > 0$. Our calculations do not confirm this suggestion. According to the results shown in Fig. 15, deformations of triaxial g-bands in, e.g., ^{104,106,108}Mo are rather stable, and it is only after the $\nu h_{11/2}$ alignment that some small reduction in β_2 is predicted. In our opinion, the decrease in the transition quadrupole moments seen experimentally is due to the mixing between a g-band and a $(\nu h_{11/2})^2$ band at $I \approx 10$. Indeed, as noted in Ref. [20], the observed moments of inertia reveal a gradual increase for $\hbar\omega$=0.2–0.4 MeV, reflecting a large-interaction band crossing. There is a difference between the TRS calculations presented in Ref. [20] and these in our study. Namely, the previous study predicts positive γ deformation for the aligned $(\nu h_{11/2})^2$ band in ^{102}Mo. In our opinion, this discrepancy is due to the different spin-orbit parameterizations employed in these two papers. As discussed in Sec. II, the spin-orbit potential used in our study was optimized to reproduce the experimental shape transition near N=56. The change in the spin-orbit strength implies a different position of the $1h_{11/2}$ neutron shell and, consequently, gives rise to a different predicted deformation pattern.

The neutron-rich *Ru isotopes* have γ-soft ground states which are stabilized by rotation (see Fig. 12). For N=60-66, the g-bands correspond to triaxial shapes with negative values

of γ. (The positive-γ minima never are predicted to be yrast at low and medium spins.) The deformation changes in ^{106}Ru due to $\nu h_{11/2}$ and $\pi g_{9/2}$ alignments are predicted to be rather small, with the g-band, $(\nu h_{11/2})^2$ band, and $(\nu h_{11/2})^2(\pi g_{9/2})^2$ band having similar deformations, $(\beta_2,\gamma)\approx(0.25, -20°)$. The strongly triaxial $(\nu h_{11/2})^4(\pi g_{9/2})^2$ configuration in ^{106}Ru becomes yrast at $I\approx40$, but it is quickly crossed by a SD band. The nuclei ^{108,110}Ru behave very similarly. Their g-bands correspond to deformation $(\beta_2,\gamma)\approx(0.28,-20°)$. The $\nu h_{11/2}$ alignment, the $\pi g_{9/2}$ alignment, and the second $\nu h_{11/2}$ alignment produce triaxial shapes with $\beta_2\approx0.2$, $\gamma\approx-45°$. The $\nu h_{11/2}$ crossing is calculated to occur at $\hbar\omega\approx0.35$ MeV for both nuclei. This is slightly lower than the observed crossing frequency, $\hbar\omega_{\rm exp}\approx0.4$ MeV [9] (see Figs. 20 and 19).

Properties of heavy Mo and Ru isotopes are often discussed in terms of triaxial degrees of freedom. Experimentally, the 2^+_2 states lie at fairly low excitation energies (≈700-800 keV), indicating the importance of γ deformation. For ^{108,110}Ru, the $B(E2)$ branching ratios measured in the γ-band at low spin are consistent with that of a rigid triaxial rotor [14]. However, it has also been pointed out that at higher spins the analysis with the rotational-vibrational model gives a better agreement [9]. More recent calculations based on the generalized collective model [82] suggest that the experimental result is consistent with the assumption of a γ-soft potential with a triaxial minimum. It should also be pointed out that the CHFB calculations with the pairing-plus-quadrupole Hamiltonian [83,84] yield triaxial shapes, and that in the interacting boson model analysis of Ref. [76] these nuclei are calculated to be near the O(6) limit rather than the SU(3) limit, thus indicating γ softness.

3. Triaxial minima with β_2=0.20–0.35, 15°$\lesssim\gamma\lesssim$45°

Triaxial minima with $\gamma>0$ are predicted at low angular momentum in the Mo and Ru isotopes. At I=0 these minima are intrinsically equivalent to the triaxial ground-state configurations with $\gamma<0$. However, due to the large moment of inertia at $\gamma<0$, the latter bands are usually favored by rotation. In most cases, the $\gamma>0$ bands have $(\beta_2,\gamma)\approx$ (0.3, 15°), and the deformation decreases to $(\beta_2,\gamma)\approx$(0.2, 30°) in the corresponding aligned configurations. An exception is the nucleus ^{100}Mo, whose yrast line has $(\beta_2,\gamma)\approx$ (0.2, 30°) up to $I\approx25$ (the negative-γ minimum quickly disappears).

At intermediate angular momentum ($I\approx$24–30, $\hbar\omega\approx$0.6–0.7 MeV) in ^{96,98,102}Sr and ^{102}Zr appear well-deformed minima appear with $(\beta_2,\gamma)\approx$ (0.2, 30°). These correspond to the aligned $(\nu h_{11/2})^4(\pi g_{9/2})^2$ configuration and become yrast or near yrast at $I\approx24$.

At very high spins ($I\approx$50–70, $\hbar\omega\approx$1.0–1.5 MeV) in ^{98,100,104,106}Zr and ^{102,106,108}Mo strongly deformed triaxial minima with β_2=0.28–0.4 and $\gamma\approx30°$ are predicted. These bands involve the $\pi h_{11/2}$ and $\nu i_{13/2}$ intruders (see Figs. 14 and 15).

4. Noncollective configurations

Noncollective many-quasi-particle states (γ=60°) correspond to the optimal (stretched) shell-model configurations with the single-particle angular momenta of all decoupled nucleons aligned along the axis of the total angular momentum. Often, the stretched states correspond to termination points of collective rotational bands. The many-quasi-particle

bands with small β_2 deformations and/or γ-values close to the γ=60° limit (seen in Figs. 13-16) are candidates for such terminating structures. (For recent calculations of terminating configurations in this mass region, see Ref. [85].)

In all nuclei considered, the TRS calculations predict that the noncollective configurations approach yrast in the spin range I=30–50. The corresponding deformations increase with increasing I, approaching $\beta_2\approx$0.3–0.35 at $I\approx$60. Since the main focus of our paper is on collective rotation and shape effects, and since the adiabatic TRS method used does not allow for a detailed description of optimal states, we do not discuss noncollective configurations quantitatively.

5. Superdeformed near-prolate minima with $\beta_2\gtrsim$0.40

The nuclei from the heavy-Zr region are excellent candidates for finding SD bands. In our calculations, SD minima have been predicted in $^{102-110}$Ru, $^{100-108}$Mo, $^{102-106}$Zr, and ^{100}Sr. These minima approach yrast at high rotational frequencies, typically at $\hbar\omega\gtrsim$0.8 MeV. Since at these high angular momenta pairing correlations are less important [105], intrinsic configurations of SD states are well characterized by the intruder orbitals carrying large principal oscillator numbers $\mathcal{N}$ (high-$\mathcal{N}$ orbitals) [107,115–117]. In this mass region, these are the $\mathcal{N}$=5 proton and $\mathcal{N}$=6 neutron states. Because of their large intrinsic angular momenta and quadrupole moments, high-$\mathcal{N}$ orbitals strongly respond to the Coriolis interaction and to the deformed average field. Consequently, their occupation numbers are good indicators of rotation and deformation properties of SD bands.

Figure 21 shows the single-particle routhian diagram representative of discussed SD configurations. The single-particle gaps in the routhian spectrum indicate the best candidates for SD bands: at low spins, the combination of the Z=42 and N=58 gaps leads to ^{100}Mo, while the Mo, Tc, and Ru isotopes with N approaching 68 are expected to favor SD high spin bands. This observation is fully corroborated by our calculations. Indeed, the $\nu 6^0\pi 5^0$ and $\nu 6^2\pi 5^2$ SD bands in ^{100}Mo and ^{110}Ru, respectively, are predicted to appear near yrast already at $I\approx$22.

For the heavy Sr isotopes, SD minima are calculated only for ^{100}Sr, and only at very high spins, $I\approx$64–70. The SD band contains two $\mathcal{N}$=6 neutrons and one $\mathcal{N}$=5 proton; hence the corresponding configuration is labeled $\nu 6^2\pi 5^1$. This configuration is also predicted in ^{102}Zr and ^{104}Zr. The corresponding SD bands behave rather smoothly with ω up to the highest spins considered. In contrast, for ^{106}Zr the SD yrast line is less regular. Here, the $\nu 6^1\pi 5^0$ band is crossed at $\hbar\omega\approx$1.1 MeV by the more strongly deformed $\nu 6^2\pi 5^1$ band. At still higher spins, there is a transition to an even more deformed structure, $\nu 6^3\pi 5^2$. The corresponding kinematic moments of inertia, $\mathcal{J}^{(1)}$, extracted from the TRS calculations are displayed in Fig. 22. It is seen that the moments of inertia in all $\nu 6^2\pi 5^1$ bands decrease gradually with frequency. The increased $\mathcal{J}^{(1)}$ in ^{106}Zr is due to the two band crossings discussed above.

At low spin, the SD minimum of the N=58 isotones of Mo and Ru (^{100}Mo and ^{102}Ru) can be associated with the configuration $\nu 6^0\pi 5^0$. At $\hbar\omega\approx$1 MeV, the configuration $\nu 6^1\pi 5^2$ becomes lower in energy (see Fig. 22). It is noted that ^{100}Mo is among the few nuclei, together with ^{108}Mo and ^{110}Ru, in which the SD minimum appears at particularly low spins, i.e., at $I\approx$20 (the corresponding SD band is calculated to appear $\approx$3 MeV above yrast). As discussed above, the microscopic reason for this structure can be explained in terms of the

SD shell gaps at Z=42 and N=58. The nuclei ^{102,104,106}Mo and ^{106,108}Ru are predicted to have rather regular SD bands associated with the $\nu 6^2 \pi 5^1$ and $\nu 6^2 \pi 5^2$ configurations. On the other hand, the SD yrast line of ^{108}Mo and ^{104}Ru is expected to be less regular, with several consecutive band crossings. The best candidates for observing high-spin SD bands in this mass region are ^{110,112}Ru.

V. CONCLUSIONS

The macroscopic-microscopic method based on the deformed Woods-Saxon potential was applied to neutron-rich nuclei from the A≈100 mass region. Thanks to a number of experimental developments, one is now able to obtain spectroscopic information on these systems, and more data should become be available in the near future, due to the large gamma-ray arrays such as GammaSphere or EuroBall, and the advent of neutron-rich radioactive beams.

The main focus of this study is on the deformation properties and shape coexistence effects at low and high angular momentum. High-spin calculations were carried out for the vacuum configurations (i.e., positive-parity, even-spin) in even-even Sr, Zr, Mo, and Ru isotopes with $58 \leq N \leq 66$.

The single-particle model used was previously optimized to reproduce the transition from spherical to deformed shapes at N≈58. The calculated ground-state deformations for heavier systems are in general agreement with experimental data.

The influence of particle number projection has been investigated. In general, the potential energy surfaces calculated with the PNP method have better developed deformed minima. A replacement of the energies at spin zero, $E^{\omega=0}$ in Eq. (3), calculated within the BCS by those calculated with PNP, has only minor consequences for predicted high-spin properties.

At low and medium spins, the alignment pattern is governed by an alignment of the $\nu h_{11/2}$ and $\pi g_{9/2}$ quasi-particles. The associated deformation changes are explained in terms of the shape polarization exerted by aligned high-j quasi-particles. According to the calculations, the first band crossing in the neutron-rich nuclei considered can be associated with the alignment of the $1h_{11/2}$ neutron pair. The frequency of the second bandcrossing, due to the $1g_{9/2}$ proton alignment, is rather high in the well-deformed Sr and Zr isotopes, but it becomes comparable with the neutron crossing frequency in the triaxial Mo and Ru isotopes.

At higher angular momenta, the high-$\mathcal{N}$ intruder orbitals, namely $\mathcal{N}$=5 protons and $\mathcal{N}$=6 neutrons, become important. They are occupied in superdeformed structures and in some highly-triaxial configurations.

From the point of view of nuclear quadrupole collectivity, probably the most interesting nuclei in the neutron-rich A≈100 mass region are systems near ^{104}Mo and ^{106}Ru, which are predicted to have stable triaxial shapes ($\gamma \approx -30°$) in 0-q.p., 2-q.p., and 4-q.p. configurations. Although the question of whether they are γ-soft or γ-deformed at low spins has not yet been settled, these systems seem to form a very good testing ground for theoretical models of nuclear triaxiality. In particular at higher spins, where the triaxial minima are predicted to be deeper, the shape with $\gamma \approx -30°$ can give rise to interesting selection rules associated with the effective C_4 symmetry of the Hamiltonian [118]. Finally, the most favorable candidates for superdeformation in this mass region are ^{100}Mo and ^{110,112}Ru in which the SD minima are predicted at particularly low spins.

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TABLES

Nucleus		Oblate			Prolate			ΔE_{op}	$\mathrm{Q_o}$	$\mathrm{Q_p}$	$\mathrm{Q_{exp}}$
Z	A	β_2	β_4	β_6	β_2	β_4	β_6	MeV	eb	eb	eb
34	56	-0.22	0.04	0.08	0.19	-0.07	0.01	0.29	-1.64	1.56	
	58	-0.25	0.05	0.09	0.21	-0.07	0.01	-0.30	-1.91	1.76	
	60	-0.28	0.06	0.09	0.22	-0.08	0.02	-1.14	-2.15	1.86	
					0.31	0.08	0.04	0.10		3.25	
	62	-0.29	0.05	0.10	0.22	-0.10	0.03	-1.36	-2.22	1.88	
					0.32	0.06	0.03	-0.20		3.31	
	64	-0.29	0.03	0.11	0.26	-0.07	0.03	-0.97	-2.20	2.28	
					0.33	0.03	0.02	0.08		3.27	
	66	-0.28	0.01	0.09	0.27	-0.07	0.03	-0.57	-2.14	2.47	
	68	-0.28	-0.02	0.08	0.29	-0.08	0.02	-0.43	-2.13	2.61	
36	56	-0.24	0.05	0.07	0.16	-0.05	0.00	-0.07	-1.93	1.40	
	58	-0.30	0.08	0.11	0.30	0.04	0.05	-0.55	-2.44	3.10	
	60	-0.31	0.07	0.10	0.32	0.04	0.04	-0.86	-2.52	3.41	
	62	-0.32	0.06	0.11	0.33	0.03	0.03	-0.81	-2.63	3.51	
	64	-0.32	0.05	0.10	0.33	0.01	0.03	-0.39	-2.61	3.52	
	66	-0.31	0.03	0.10	0.33	-0.02	0.04	-0.06	-2.56	3.39	
	68	-0.31	0.00	0.09	0.32	-0.05	0.04	0.11	-2.52	3.28	
	70	-0.31	-0.01	0.08	0.31	-0.07	0.03	0.06	-2.59	3.16	
	72	-0.32	0.00	0.06	0.30	-0.06	0.02	0.25	-2.71	3.01	
38	56	-0.11	-0.03	0.00	0.27	0.04	0.04	-0.85	-0.92	2.96	
	58	-0.28	0.05	0.07	0.33	0.04	0.04	0.41	-2.40	3.70	
	60	-0.33	0.07	0.10	0.34	0.04	0.03	0.49	-2.81	3.84	3.12
	62	-0.34	0.07	0.11	0.35	0.03	0.02	0.64	-2.96	3.98	3.32
	64	-0.34	0.06	0.11	0.36	0.01	0.01	1.10	-2.98	4.04	
	66	-0.32	0.03	0.09	0.35	-0.01	0.02	1.48	-2.84	3.97	
	68	-0.30	-0.01	0.07	0.35	-0.04	0.03	1.48	-2.64	3.87	
	70	-0.30	-0.03	0.06	0.35	-0.05	0.02	1.38	-2.65	3.88	
	72	-0.32	-0.01	0.06	0.36	-0.05	0.02	1.22	-2.83	4.06	

TABLE I. Calculated equilibrium deformations β_2, β_4, and β_6 of the ground-state and excited minima in neutron-rich even-even Se-Cd isotopes. The energy differences between the local minima, and the corresponding quadrupole moments are also shown, together with experimental quadrupole moments [109].

Nucleus		Oblate			Prolate			ΔE_{op}	Q_o	Q_p	Q_{exp}
Z	A	β_2	β_4	β_6	β_2	β_4	β_6	MeV	eb	eb	eb
40	56				0.00	0.00	0.00			0.00	0.74
	58	-0.17	-0.02	-0.01	0.29	0.05	0.02	-0.05	-1.60	3.40	
	60	-0.21	-0.01	0.01	0.34	0.03	0.00	0.85	-2.01	4.09	3.01
	62	-0.24	0.00	0.01	0.36	0.02	-0.01	1.51	-2.25	4.37	4.01
	64	-0.25	-0.02	0.02	0.37	0.00	-0.01	1.67	-2.33	4.45	
	66	-0.24	-0.04	0.01	0.37	-0.02	-0.01	1.42	-2.25	4.37	
	68	-0.25	-0.06	0.01	0.36	-0.05	0.00	1.02	-2.26	4.23	
	70	-0.25	-0.07	0.01	0.36	-0.06	0.00	0.84	-2.28	4.24	
	72	-0.22	-0.08	-0.01	0.38	-0.06	-0.01	0.45	-2.05	4.59	
	74	-0.18	-0.09	-0.03	0.37	-0.05	-0.01	-0.90	-1.70	4.50	
42	58	-0.18	-0.02	0.00	0.00	0.00	0.00	0.01	-1.79	0.00	2.28
					0.20	0.05	0.01	0.05		2.42	
	60	-0.21	-0.02	0.00	0.27	0.05	0.01	0.22	-2.08	3.46	3.26
					0.34	0.02	-0.03	0.30		4.27	
	62	-0.23	-0.03	0.00	0.35	0.03	-0.02	0.60	-2.23	4.51	3.29
	64	-0.24	-0.05	0.00	0.38	0.02	-0.03	0.58	-2.29	4.91	3.62
	66	-0.24	-0.06	0.00	0.38	-0.01	-0.02	0.13	-2.32	4.86	3.68
	68	-0.25	-0.08	0.00	0.33	-0.04	0.00	-0.49	-2.40	4.15	
	70	-0.25	-0.09	0.00	0.33	-0.06	0.00	-0.91	-2.36	4.02	
	72	-0.23	-0.09	-0.01	0.28	-0.05	0.00	-1.42	-2.27	3.49	
					0.42	-0.05	-0.01	-0.07		5.45	
	74	-0.21	-0.10	-0.03	0.21	-0.03	0.01	-2.22	-2.00	2.67	
44	60	-0.21	-0.02	-0.01	0.22	0.05	0.00	0.62	-2.18	2.88	2.91
	62	-0.23	-0.03	-0.01	0.25	0.04	-0.01	0.45	-2.40	3.40	
	64	-0.24	-0.05	0.00	0.26	0.03	-0.01	0.15	-2.45	3.54	3.22
	66	-0.24	-0.07	0.00	0.26	0.01	-0.01	-0.36	-2.47	3.41	3.34
	68	-0.25	-0.09	0.00	0.25	-0.02	0.00	-0.88	-2.51	3.30	3.36
	70	-0.25	-0.09	0.00	0.24	-0.03	0.00	-1.19	-2.52	3.17	
	72	-0.24	-0.10	-0.01	0.22	-0.04	0.00	-1.43	-2.41	2.89	
	74	-0.21	-0.11	-0.03	0.17	-0.02	0.00	-1.58	-2.12	2.21	
	76	-0.18	-0.11	-0.04	0.08	0.00	0.00	-1.31	-1.90	1.11	
					0.51	0.04	0.05	5.08		8.05	

TABLE I. (Continued)

Nucleus		Oblate			Prolate			ΔE_{op}	$\mathrm{Q_o}$	$\mathrm{Q_p}$	$\mathrm{Q_{exp}}$
Z	A	β_2	β_4	β_6	β_2	β_4	β_6	MeV	eb	eb	eb
46	56				0.02	0.01	0.00			0.21	2.15
	58				0.14	0.03	-0.01			1.89	2.32
	60				0.18	0.03	-0.01			2.42	2.57
	62	-0.23	-0.01	-0.01	0.21	0.04	-0.01	1.00	-2.60	2.97	2.76
	64	-0.24	-0.03	-0.01	0.22	0.03	-0.01	0.74	-2.63	3.11	2.96
	66	-0.24	-0.05	0.00	0.21	0.00	0.00	0.37	-2.64	2.91	2.52
	68	-0.24	-0.07	0.00	0.21	-0.02	0.00	0.00	-2.66	2.82	1.84
	70	-0.24	-0.08	0.00	0.20	-0.03	0.00	-0.20	-2.65	2.77	2.40
	72	-0.23	-0.08	-0.01	0.18	-0.03	0.00	-0.24	-2.54	2.47	
	74	-0.19	-0.09	-0.03	0.14	-0.02	0.00	-0.16	-2.12	1.91	
	76	-0.13	-0.07	-0.03	0.12	-0.01	0.00	-0.07	-1.56	1.61	
					0.51	0.03	0.06	7.52		8.40	
	78	0.00	0.00	0.00	0.54	0.03	0.05	-9.25	0.03	9.07	
48	56				0.00	0.00	0.00			0.00	
	58				0.03	0.00	0.00			0.43	2.03
	60	-0.04	0.00	0.00	0.12	0.01	0.00	0.24	-0.50	1.66	2.08
	62	-0.07	0.01	0.00	0.15	0.00	0.00	0.42	-0.90	2.07	2.13
	64	-0.09	0.01	0.00	0.17	0.01	0.00	0.52	-1.18	2.49	2.26
	66	-0.10	0.00	0.00	0.18	-0.01	0.01	0.57	-1.34	2.61	2.35
	68	-0.11	-0.01	0.00	0.17	-0.03	0.01	0.56	-1.37	2.41	2.37
	70	-0.10	-0.01	0.00	0.16	-0.03	0.01	0.48	-1.25	2.31	
	72	-0.08	-0.02	0.00	0.14	-0.03	0.01	0.24	-1.09	1.96	
	74	-0.07	-0.02	-0.01	0.09	-0.02	0.00	0.07	-0.90	1.28	
	76				0.00	0.00	0.00			-0.03	

TABLE I. (Continued)

		PNP				BCS			
Z	N	β_2	β_4	γ	Q_{cal}	β_2	β_4	γ	Q_{cal}
42	58	0.210	0.011	-32.726	3.008	0.162	0.001	-51.801	2.103
	60	0.300	0.035	0.000	3.973	0.243	0.019	-20.538	3.547
	62	0.316	0.017	-19.046	4.737	0.291	0.021	-14.055	4.261
	64	0.335	0.016	-19.695	5.116	0.308	0.015	-16.866	4.619
	66	0.328	0.001	-21.119	5.008	0.306	0.005	-18.690	4.629
44	58	0.231	0.015	-25.030	3.541	0.125	0.013	0.000	1.606
	60	0.252	0.019	-23.157	3.940	0.184	0.020	0.000	2.460
	62	0.275	0.003	-19.507	4.271	0.245	0.003	-18.232	3.756
	64	0.284	0.014	-19.875	4.533	0.263	0.013	-21.254	4.185
	66	0.283	0.004	-21.870	4.550	0.272	0.012	-23.660	4.413

TABLE II. Equilibrium deformations β_2, γ, and β_4 and corresponding quadrupole moments (in eb) for the Mo and Ru isotopes calculated in the PNP (left) and BCS (right) variants.

FIGURES

FIG. 1. Single particle neutron (top) and proton (bottom) levels of the deformed Woods-Saxon potential as a function of quadrupole deformation β_2. Positive (negative) parity states are indicated by solid (dotted) lines, and the spherical and deformed shell and subshell closures are indicated. Calculations are performed with the Woods-Saxon set of parameters of Ref. [36] corresponding to the central nucleus ^{100}Zr.

FIG. 2. Potential-energy curves for the even-even neutron-rich isotopes of Kr, Sr, and Zr obtained in the FRLD/PNP (left) and FRLD/BCS (right) variant of calculations. At each value of β_2, the energy has been minimized with respect to deformations β_4 and β_6.

FIG. 3. Same as in Fig. 2 except for the even-even neutron-rich isotopes of Mo, Ru, and Pd.

FIG. 4. Total energy surfaces in the (β_2, γ)-plane for ^{100,102}Zr, in the LD/PNP (left) and LD/BCS (right) variant of calculations. At each mesh point (β_2, γ) the total energy has been minimized with respect to β_4. The distance between thick contour lines is 1 MeV, while between the thin contour line it is 250 keV.

FIG. 5. Same as in Fig. 4 except for ^{104,106}Zr.

FIG. 6. Same as in Fig. 4 except for ^{100,102}Mo.

FIG. 7. Same as in Fig. 4 except for ^{104,106}Mo.

FIG. 8. Same as in Fig. 4 except for ^{104,106}Ru.

FIG. 9. Same as in Fig. 4 except for ^{108,110}Ru.

FIG. 10. Total routhian surfaces in the (β_2, γ)-plane for the (π=+, r=1) quasi-particle vacuum configuration of ^{100}Sr at four values of rotational frequency: $\hbar\omega$=0.3, 0.6, 0.9, and 1.2 MeV. At each (β_2, γ) point the total routhian has been minimized with respect to hexadecapole deformation β_4. The distance between thick contour lines is 1 MeV, while between the thin contour line it is 250 keV. The angular momentum values at local minima are indicated.

FIG. 11. Same as in Fig. 10 except for ^{102}Zr.

FIG. 12. Same as in Fig. 10 except for ^{108}Ru.

FIG. 13. Summary of calculated equilibrium deformations of yrast and near-yrast (π=+, r=1) bands in ^{96,98,100,102,104}Sr. The rotational frequency is varied from $\hbar\omega$=0 to $\hbar\omega$=1.5 MeV, with steps of $\Delta\omega$=0.07 MeV/$\hbar$. If the two minima corresponding to the TRS's calculated at ω and $\omega+\Delta\omega$ have the same intrinsic configuration, and the change in equilibrium deformation is small, $\Delta(\beta_2 \cos\gamma) \leq 0.1$, they are assumed to belong to the same rotational band and they are connected by a solid line. Whenever feasible, the direction of increasing ω is marked by an arrow. The symbols indicating the intrinsic configuration are put at the lowest and highest frequency at which the band is calculated, and the corresponding spin range is shown by numbers. The legend displays band labels. Superdeformed bands and high-spin bands with γ>0 are classified according to the number of occupied high-$\mathcal{N}$ intruder levels ($\mathcal{N}$ = 6 and 5 for neutrons and protons, respectively). Other band structures are classified according to the number of aligned high-j quasi-particles: $\nu h_{11/2}$, $\pi g_{9/2}$, and $\nu i_{13/2}$.

FIG. 14. Same as in Fig. 13 except for ^{98,100,102,104,106}Zr.

FIG. 15. Same as in Fig. 13 except for ^{100,102,104,106,108}Mo.

FIG. 16. Same as in Fig. 13 except for ^{102,104,106,108,110}Ru.

FIG. 17. Single quasi-particle routhian diagram for N=62 (top) and Z=40 (bottom) at β_2=0.3 and γ=0°. This diagram is typical for the well-deformed prolate bands in the heavy-Zr region. The parity and signature of individual levels are indicated in the following way: π=+, r=$-i$ - solid line; π=+, r=+i - dotted line; π=–, r=$-i$ - dot-dashed line; π=–, r=+i - dashed line. The thin line indicates the Fermi energy.

FIG. 18. Experimental and calculated angular momentum alignment for yrast bands of well-deformed ^{100,102}Zr. Experimental data are taken from Ref. [19]. The diabatic bands have not been extracted in the calculation. Therefore, the band crossing region is not reproduced theoretically.

FIG. 19. Single quasi-particle routhian diagram for N=64 (top) and Z=44 (bottom) at β_2=0.23 and γ=–30°. This diagram is typical for the triaxial bands in the heavy-Mo region. The line characteristics have the same interpretation as in Fig. 17.

FIG. 20. Experimental and calculated angular momentum alignment for triaxial yrast line in ^{108}Ru. Experimental data are taken from Ref. [9]. The diabatic bands have not been extracted in the calculation. Therefore, the band crossing region is not reproduced theoretically.

FIG. 21. Single-particle routhian diagram for neutrons (top) and protons (bottom) at β_2=0.45 and γ=0°, characteristic of SD configurations in the heavy Zr region. The line convention is the same as in Fig. 17.

FIG. 22. Calculated kinematic moments of inertia versus rotational frequency for superdeformed bands in even-even nuclei around ^{104}Mo. The symbols indicate the same configurations as in Figs. 13-16.

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